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# An optimal algorithm and superrelaxation for minimization of a quadratic function subject to separable convex constraints with applications

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**Abstract** We propose a modification of our MPGP algorithm for the solution of bound constrained quadratic programming problems so that it can be used for minimization of a strictly convex quadratic function subject to separable convex constraints. Our active set based algorithm explores the faces by conjugate gradients and changes the active sets and active variables by gradient projections, possibly with the superrelaxation steplength. The solution error in terms of extreme eigenvalues guarantees that if a class of problems has the spectrum of the Hessian matrix in a given positive interval, then the algorithm can find and recognize an approximate solution of any particular problem in a number of iterations that is uniformly bounded. We also show how to use the algorithm for the solution of separable and equality constraints. The power of our algorithm and its optimality demonstrated on the solution of two cantilever beams in mutual contact with Tresca friction discretized by more than four millions nodal variables.

**Keywords** QPQC with separable constraints · spherical constraints · rate of convergence

**Mathematics Subject Classification (2000)** 65K10 · 90C20 · 90C25 · 90C90

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## 1 Introduction

We are interested in the problem to find

$$\min_{x\in\Omega} f(x), \tag{1}$$

where $f = \frac{1}{2}x^T Ax - x^T b$, $A \in \mathbb{R}^{n\times n}$ denotes a symmetric positive definite matrix, $b, x \in \mathbb{R}^n$,

$$x = [\mathbf{x}_1^T, \ldots, \mathbf{x}_s^T]^T, \quad \mathbf{x}_i \in \mathbb{R}^{\ell_i}, \quad \ell_1 + \cdots + \ell_s = n,$$

and

$$\Omega = \Omega_1 \times \cdots \times \Omega_s$$

denotes a closed convex set defined by differentiable functions $h_i : \mathbb{R}^{\ell_i} \to \mathbb{R}$, $i = 1, \ldots, s$, so that

$$\Omega_i = \{\mathbf{x}_i \in \mathbb{R}^{\ell_i} : h_i(\mathbf{x}_i) \leq 0\}, \ i = 1, \ldots, s.$$

An important special case of (1) is minimization subject to spherical constraints

$$h_i(\mathbf{x}_i) = \|\mathbf{x}_i - \mathbf{z}_i\|^2 - r_i^2, \quad \mathbf{z}_i \in \mathbb{R}^{\ell_i}, \ r_i > 0. \tag{2}$$

For $\ell_i = 1$, we get the box constraints

$$l_i \leq x_i \leq u_i, \quad l_i = z_i - r_i, \quad u_i = z_i + r_i,$$

for $\ell_i = 1$ and both $r_i$ and $z_i$ sufficiently large, we can mimic the bound constraints

$$l_i \leq x_i, \quad l_i = z_i - r_i,$$

and for $\ell_i = 1$ and $r_i$ sufficiently large, we can mimic $\Omega_i = \mathbb{R}^{\ell_i}$. We suppose that $\Omega$ is non-empty, and, in order to avoid unnecessary complications, we assume that $h_i(\mathbf{x}_i) = 0$ implies $\nabla h_i(\mathbf{x}_i) \neq 0$. To enable applications of a stopping criterion , we assume $b \neq 0$.

Motivated by our recent development of scalable algorithms for variational inequalities (Dostál [13], Bouchala, Dostál, Sadowská [4], and Dostál et al. [18]), we are interested especially in the algorithms with nontrivial bounds on the decrease of $f$ in terms of bounds on the spectrum of the Hessian matrix $A$. While such results are standard for the solution of unconstrained quadratic programming problems (see, e.g., Saad [37]), it seems that until recently there were no such results for inequality constrained problems. The standard results either provide bounds on the contraction of the gradient projection [3], or guarantee only some qualitative properties of convergence (see, e.g., Conn, Gould, and Toint for the trust region methods [8], Ben–Tal and Nemirovski for conic programming [2], and Ecker and Niemi [21], Martínez [32], Anitescu [1], or Mehrotra and Sun [34] for some QPQC algorithms). Luo and Tseng proved in [30] and [31] the linear rate of convergence of the cost function for the gradient projection method, but they did not make any attempt to specify the constants.

It seems that the first step in the development of the algorithms that we are interested in was carried out by Schöberl [38], who found a bound on the decrease of a quadratic cost function for the gradient projection set defined by bound constraints with the steplength $\alpha \in (0, 1/\|A\|]$. Later he improved his original estimate [20]. The result was exploited in the analysis of the rate of convergence of the active set based algorithm for bound constrained quadratic programming which combined the conjugate

Mathematical programming. 2012, vol. 135, no. 1-2, p. 195-220. http://dx.doi.org/10.1007/s10107-011-0454-2



gradient method with the fixed steplength gradient projection and proportioning [20]. The drawback of these results was their restriction to the steplength $\alpha \in (0, 1/\|A\|]$, while the best performance was observed for $\alpha \in (1/\|A\|, 2/\|A\|]$. The gap in the theory has been filled in only recently by Dostál [12] and Dostál, Domorádová, and Sadowská [14].

While the results mentioned above were formulated only for bound constrained problems, the proof of the original estimate for $\alpha \in (0, 1/\|A\|]$ by Schöberl uses only the convexity of a feasible set and is valid for any convex constraints. Though this is not true for the estimate for $\alpha \in (1/\|A\|, 2/\|A\|]$ [12], a closer examination of the proof of the superrelaxation estimate reveals that it is based on a simple geometric property of the half-interval that can be generalized to some other convex sets that we call subsymmetric [5]. The point of this note is to use the latter result to modify our MPGP algorithm [13] so that it can be used to the solution of some important instances of (1) and to show that the algorithm can solve effectively large problems such as those arising from the discretization of contact problems with friction.

Our research offers an alternative to the approach of Kučera (see [28], [29], and [19]), who was the first to observe that the above results by Schöberl and Dostál can be adapted to the solution of (1). There are three main innovations in this paper. First, we introduce a natural generalization of the projected gradient, which is well-known from the bound constrained quadratic programming, and use it in our development. The second innovation concerns the difference between problem (1) and the bound constrained problems, in particular that the knowledge of the active set of the solution of (1) need not reduce it to a linear problem. Here we propose a strategy which takes this observation into account by invoking more often the gradient projection. The third innovation comprises superrelaxation based on recent results on the projections onto the so called subsymmetric sets [5]. We also show that our generalization of the projected gradient natural inequalities that are valid for the standard projected gradient for bound constrained problems.

The paper is organized as follows. After recalling some basic concepts and notations, we introduce in Section 3 a generalization of the projected gradient and show that it can be used to define quantitative refinement of the Karush–Kuhn–Tucker (KKT) conditions. In Section 4, we present our MPGP algorithm in the form that is suitable for analysis. In Sections 5 and 6, we give the R-linear bounds on the decrease of the cost function and on the norm of the projected gradient, respectively. Application of MPGP to the solution of problems with convex separable inequality constraints and linear equality constraints is briefly described in Section 7. The algorithm is tested on numerical solution of a coercive contact problem with friction in Section 8. Some comments on possible generalizations can be found in the last section.

## 2 Notations and preliminaries

Let us introduce some conventions that we use throughout the whole paper. If $v \in \mathbb{R}^n$ is a vector, then $v_j \in \mathbb{R}$ denotes its $j$-th entry, $1 \leq j \leq n$, $\mathbf{v}_i \in \mathbb{R}^{\ell_i}$ is its $i$-th segment, $1 \leq i \leq s$, and $v = (\mathbf{v}_1^T, \ldots, \mathbf{v}_s^T)^T$; the integers $\ell_i$ are given by the formulation of problem (1). For any non-empty set of indices $\mathcal{I}$ and a vector $x \in \mathbb{R}^n$, we denote by

$x_{\mathcal{I}}$ a subvector of $x$ with the entries given by $\mathcal{I}$. In particular, $\mathbf{v}_i = v_{\mathcal{I}_i}$ with

$$\mathcal{I}_i = \{\sum_{k=1}^{i-1} \ell_k + 1, \dots, \sum_{k=1}^{i} \ell_k\}.$$

The Euclidean norm of $v \in \mathbb{R}^p$ is denoted by

$$\|v\| = (v_1^2 + \cdots + v_p^2)^{1/2}$$

and the same notation is used for the induced matrix norm. Similarly, if $M$ is a symmetric positive definite matrix, then the norm of $v$ associated with the scalar product defined by $M$ is given by

$$\|v\|_M^2 = v^T M v.$$

The eigenvalues of the Hessian $A$ of $f$ are denoted by $\lambda_i(A)$,

$$\lambda_{\min}(A) = \lambda_1(A) \leq \cdots \leq \lambda_n(A) = \lambda_{\max}(A) = \|A\|.$$

The set of all eigenvalues is denoted by $\sigma(A)$ and it is called the spectrum of $A$. The spectral condition number $\kappa(A)$ of $A$ is given by

$$\kappa(A) = \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)}.$$

The gradient $g = g(x)$ of $f$ at $x \in \mathbb{R}^n$ is defined by

$$g = g(x) = Ax - b = \nabla f(x).$$

We assume that $b$ and $g$ have the same block structure as $x$, i.e.,

$$b = [\mathbf{b}_1^T, \dots, \mathbf{b}_s^T]^T, \quad \mathbf{b}_i \in \mathbb{R}^{\ell_i}, \quad g = [\mathbf{g}_1^T, \dots, \mathbf{g}_s^T]^T, \quad \mathbf{g}_i \in \mathbb{R}^{\ell_i}.$$

In what follows, we denote by $P_\Omega$ the Euclidean projection to $\Omega$, so that

$$P_\Omega(x) = \arg\min_{y \in \Omega} \|x - y\|.$$

Since the constraints that define $\Omega$ are separable, we can define $P_\Omega$ block-wise by

$$P_{\Omega_i}(\mathbf{x}_i) = \arg\min_{\mathbf{y} \in \Omega_i} \|\mathbf{x}_i - \mathbf{y}\|, \quad P_\Omega(x) = \left[P_{\Omega_1}(\mathbf{x}_1)^T, \dots, P_{\Omega_s}(\mathbf{x}_s)^T\right]^T. \tag{3}$$

To extend our earlier results concerning the bound constrained problems [12], recall that the estimate of the decrease of the cost function $f$ along the projected-gradient path for $\Omega$ defined by bound constraints was based on a special property of the set $\Omega = (-\infty, a]$, $a \in \mathbb{R}$. The property can be conveniently characterized in terms of geometry as in the following definition.

**Definition 2.1** *A closed convex set $\Omega \subseteq \mathbb{R}^n$ is* subsymmetric *if for any $x \in \Omega$, $y \in \mathbb{R}^n$, $g = x - y$, and $\tau \in [0, 1]$*

$$\|P_\Omega(y + \tau g) - y\| \geq \|P_\Omega(y - \tau g) - y\|. \tag{4}$$

For illustration see Fig. 1.

Mathematical programming. 2012, vol. 135, no. 1-2, p. 195-220. http://dx.doi.org/10.1007/s10107-011-0454-2



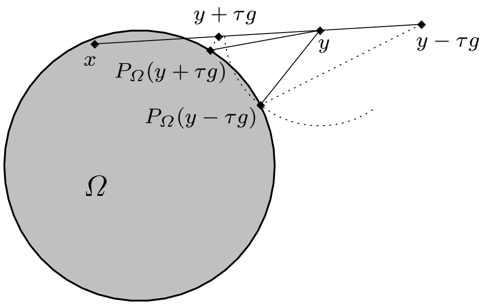


**Fig. 1** The condition which defines a subsymmetric set.

## 3 Projected gradient and quantitative refinement of KKT conditions

It is well known that the solution to problem (1) always exists, and it is necessary unique [3]. The unique solution $\widehat{x}$ of (1) is fully determined by the KKT conditions [3], so that there is $\lambda \in \mathbb{R}^s$ such that

$$\widehat{\mathbf{g}}_i + \nabla h_i(\widehat{\mathbf{x}}_i)\lambda_i = \mathbf{o}, \quad h_i(\widehat{\mathbf{x}}_i)\lambda_i = 0, \quad \lambda_i \geq 0, \quad \text{and} \quad h_i(\widehat{\mathbf{x}}_i) \leq 0, \; i = 1, \ldots, s, \tag{5}$$

where we use the notation $\widehat{g} = g(\widehat{x})$.

To give a quantitative refinement of the KKT conditions (5), we begin with some notations. Let $\mathcal{S}$ denote the set of all indices of the constraints so that

$$\mathcal{S} = \{1, 2, \ldots, s\}.$$

For any $x \in \mathbb{R}^n$, we call an *active set* of $x$ the set of all indices for which $h_i(\mathbf{x}_i) = 0$. We denote it by $\mathcal{A}(x)$ so that

$$\mathcal{A}(x) = \{i \in \mathcal{S} : h_i(\mathbf{x}_i) = 0\}.$$

Its complement

$$\mathcal{F}(x) = \{i \in \mathcal{S} : h_i(\mathbf{x}_i) \neq 0\}$$

is called a *free set*.

For $x \in \Omega$, we define the outer unit normal $n$ by

$$\mathbf{n}_i = \mathbf{n}_i(x) = \begin{cases} \|\nabla h_i(\mathbf{x}_i)\|^{-1} \nabla h_i(\mathbf{x}_i) & \text{for} \quad i \in \mathcal{A}(x), \\ \mathbf{o} \quad \text{for} \quad i \in \mathcal{F}(x). \end{cases}$$

The components of the gradient that violate the KKT conditions (5) in the free set and active set are called the *free gradient* $\varphi$ and the *chopped gradient* $\beta$, respectively. They are defined by

$$\boldsymbol{\varphi}_i(x) = \mathbf{g}_i(x) \text{ for } i \in \mathcal{F}(x), \qquad \boldsymbol{\varphi}_i(x) = \mathbf{o} \text{ for } i \in \mathcal{A}(x), \tag{6}$$

$$\boldsymbol{\beta}_i(x) = \mathbf{o} \text{ for } i \in \mathcal{F}(x), \qquad \boldsymbol{\beta}_i(x) = \mathbf{g}_i(x) - \{\mathbf{n}_i^T \mathbf{g}_i\}^- \mathbf{n}_i \text{ for } i \in \mathcal{A}(x), \tag{7}$$

where we use the notation

$$\{\mathbf{n}_i^T \mathbf{g}_i\}^- = \min\{\mathbf{n}_i^T \mathbf{g}_i, 0\}.$$

Mathematical programming. 2012, vol. 135, no. 1-2, p. 195-220. http://dx.doi.org/10.1007/s10107-011-0454-2



Thus the KKT conditions (5) are satisfied if and only if the *projected gradient*

$$g^P(x) = \varphi(x) + \beta(x)$$

is equal to zero.

Since

$$\mathbf{g}_i^P(x) = \mathbf{g}_i(x), \quad i \in \mathcal{F}(x),$$

and for any $i \in \mathcal{A}(x)$

$$\begin{aligned}\|\mathbf{g}_i^P\|^2 &= \|\boldsymbol{\beta}_i\|^2 = (\mathbf{g}_i - \{\mathbf{n}_i^T\mathbf{g}_i\}^-\mathbf{n}_i)^T(\mathbf{g}_i - \{\mathbf{n}_i^T\mathbf{g}_i\}^-\mathbf{n}_i)\\ &= \|\mathbf{g}_i\|^2 - \left(\{\mathbf{n}_i^T\mathbf{g}_i\}^-\right)^2 = \mathbf{g}_i^T\mathbf{g}_i^P,\end{aligned}$$

we have

$$\|g^P\|^2 = g^Tg^P \le \|g\|\,\|g^P\| \tag{8}$$

and

$$\|g^P\| \le \|g\|. \tag{9}$$

We need yet another simple property of the projected gradient.

**Lemma 1** *Let $x, y \in \Omega$ and $g = \nabla f(x)$. Then*

$$g^T(y-x) \ge (g^P)^T(y-x). \tag{10}$$

*Proof* First observe that

$$g^T(y-x) = (g-g^P)^T(y-x) + (g^P)^T(y-x).$$

Using the definition of the projected gradient, we get

$$(g-g^P)^T(y-x) = \sum_{i\in\mathcal{S}}(\mathbf{g}_i - \mathbf{g}_i^P)^T(\mathbf{y}_i - \mathbf{x}_i) = \sum_{i\in\mathcal{A}(x)}\{\mathbf{n}_i^T\mathbf{g}_i\}^-\mathbf{n}_i^T(\mathbf{y}_i - \mathbf{x}_i).$$

To finish the proof, it is enough to observe that for $i \in \mathcal{A}(x)$

$$\mathbf{n}_i^T(\mathbf{y}_i - \mathbf{x}_i) \le 0$$

due to the convexity of $\Omega_i$.

The following lemma can be considered as a quantitative refinement of the KKT conditions.

**Lemma 2** *Let $\widehat{x}$ be the solution of (1) and let $g^P = g^P(x)$ denote the projected gradient at $x \in \Omega$. Then*

$$\|x-\widehat{x}\|_A^2 \le 2\big(f(x) - f(\widehat{x})\big) \le \|g^P\|_{A^{-1}}^2. \tag{11}$$

Mathematical programming. 2012, vol. 135, no. 1-2, p. 195-220. http://dx.doi.org/10.1007/s10107-011-0454-2



*Proof* Let $\widehat{\mathcal{A}}$, $\widehat{\mathcal{F}}$, and $\widehat{g}$ denote the active set, free set, and the gradient at the solution, respectively. Observe that if $i \in \widehat{\mathcal{A}}$ and $\mathbf{x}_i \in \Omega_i$, then, using the convexity of $h_i$,

$$\left(\nabla h_i(\widehat{\mathbf{x}}_i)\right)^T (\mathbf{x}_i - \widehat{\mathbf{x}}_i) \leq h_i(\mathbf{x}_i) - h_i(\widehat{\mathbf{x}}_i) = h_i(\mathbf{x}_i) \leq 0.$$

It follows by the KKT conditions (5) and $\widehat{g}_{\widehat{\mathcal{F}}} = o_{\widehat{\mathcal{F}}}$ that

$$\widehat{g}^T(x - \widehat{x}) = \sum_{i \in \widehat{\mathcal{A}}} \widehat{\mathbf{g}}_i^T (\mathbf{x}_i - \widehat{\mathbf{x}}_i) = \sum_{i \in \widehat{\mathcal{A}}} -\lambda_i \left(\nabla h_i(\widehat{\mathbf{x}}_i)\right)^T (\mathbf{x}_i - \widehat{\mathbf{x}}_i) \geq 0. \tag{12}$$

Thus, for any $x \in \Omega$,

$$f(x) - f(\widehat{x}) = \widehat{g}^T(x - \widehat{x}) + \frac{1}{2}(x - \widehat{x})^T A (x - \widehat{x}) \geq \frac{1}{2}\|x - \widehat{x}\|_A^2.$$

This proves the left inequality of (11).

To prove the right inequality, we can use Lemma 1 and simple manipulations to get for any $x \in \Omega$

$$\begin{aligned} 0 \geq 2\big(f(\widehat{x}) - f(x)\big) &= \|\widehat{x} - x\|_A^2 + 2g^T(\widehat{x} - x) \\ &\geq \|\widehat{x} - x\|_A^2 + 2\left(g^P\right)^T(\widehat{x} - x) \\ &\geq 2 \min_{y \in \mathbb{R}^n} \left(\frac{1}{2} y^T A y + \left(g^P\right)^T y\right) = -(g^P)^T A^{-1} g^P. \end{aligned}$$

The right inequality of (11) now follows easily.

## 4 MPGP algorithm

The algorithm that we propose here exploits a user-defined constant $\delta \in (0, 1/2]$, a test which is used to decide when to change the face, and two types of steps.

The *conjugate gradient step* is defined by

$$x^{k+1} = x^k - \alpha_{cg} p^{k+1}, \quad \alpha_{cg} = b^T p^{k+1} / p^{k+1} A p^{k+1}, \tag{13}$$

where $p^{k+1}$ is the conjugate gradient direction (see, e.g. Saad [37] or Dostál [13]) which is constructed recurrently. The recurrence starts (or restarts) with $p^{k+1} = \varphi(x^k)$ whenever $x^k$ is generated by the gradient projection step. If $x^k$ is generated by the conjugate gradient step, then $p^{k+1}$ is given by the formulae

$$p^{k+1} = \varphi(x^k) - \gamma p^k, \quad \gamma = \frac{\varphi(x^k)^T A p^k}{(p^k)^T A p^k}. \tag{14}$$

The coefficient $\alpha_{cg}$ is chosen so that

$$\begin{aligned} f(x^{k+1}) &= \min\{f\big(x^k - \alpha p^{k+1}\big) : \alpha \in \mathbb{R}\} \\ &= \min\{f(x) : x \in x^r + \mathrm{Span}\big(p^{r+1}, \ldots, p^{k+1}\big), \end{aligned}$$

Mathematical programming. 2012, vol. 135, no. 1-2, p. 195-220. http://dx.doi.org/10.1007/s10107-011-0454-2



where $\mathrm{Span}\big(p^{r+1},\dots,p^{k+1}\big)$ denotes the smallest subspace of the vector space $\mathbb{R}^n$ which includes $p^{r+1},\dots,p^{k+1}$ and $x^r$ denotes the last iterate generated by the gradient projection step. It can be checked directly that

$$f(x^{k+1}) \le f\left(x^k - \alpha_{cg}\varphi(x^k)\right) = f(x^k) - \frac{1}{2}\frac{\|\varphi(x^k)\|^4}{\varphi(x^k)^T A\varphi(x^k)}. \tag{15}$$

The conjugate gradient steps are used to speed up the minimization in the face

$$\mathcal{W}_{\mathcal{J}} = \{x : h_i(\mathbf{x}_i) = 0, \quad i \in \mathcal{J}\}, \quad \mathcal{J} = \mathcal{A}(x^r).$$

The *gradient projection step* is defined by the gradient projection

$$x^{k+1} = P_\Omega\big(x^k - \alpha g(x^k)\big) \tag{16}$$

with the fixed steplength $\alpha > 0$. This step can both add and remove the indices from the current working set. To describe the gradient projection step in the form suitable for our analysis, let us introduce, for any $x \in \Omega$ and $\alpha > 0$, the *reduced gradient* $\widetilde{g} = \widetilde{g}_\alpha(x)$

$$\widetilde{g} = \frac{1}{\alpha}\big(x - P_\Omega(x - \alpha g)\big) \tag{17}$$

and its components, the *reduced free gradient* $\widetilde{\varphi} = \widetilde{\varphi}_\alpha(x)$ and the *reduced chopped gradient* $\widetilde{\beta} = \widetilde{\beta}_\alpha(x)$ by

$$\begin{aligned} &\widetilde{\boldsymbol{\varphi}}_i = \widetilde{\mathbf{g}}_i \ \text{ for } \ i \in \mathcal{F}(x), \quad &&\widetilde{\boldsymbol{\varphi}}_i = \mathbf{o} \ \text{ for } \ i \in \mathcal{A}(x),\\ &\widetilde{\boldsymbol{\beta}}_i = \mathbf{o} \ \text{ for } \ i \in \mathcal{F}(x), \quad &&\widetilde{\boldsymbol{\beta}}_i = \widetilde{\mathbf{g}}_i \ \text{ for } \ i \in \mathcal{A}(x). \end{aligned}$$

If the steplength is equal to $\alpha$ and given $\delta \in (0, 1/2]$ the inequality

$$2\delta g^T g^P \le \|\varphi(x^k)\|^2 \tag{18}$$

holds, then we call the iterate $x^k$ *proportional*. The test (18) is used to decide which component of the projected gradient $g^P(x^k)$ should be reduced in the next step. The test can be written also in the form

$$\|\beta(x^k)\| \le \Gamma\|\varphi(x^k)\|, \quad \Gamma^2 = \frac{1-2\delta}{2\delta}. \tag{19}$$

Similar tests were used in the algorithms for the bound constrained quadratic programming problems introduced independently by Friedlander and Martínez with their collaborators (see [22] or [23]) and Dostál [9]. Notice that for $\delta = 1/4$ we get $\Gamma = 1$, the choice which tries to reduce the free gradient by the conjugate gradient step when $\|\varphi(x^k)\| \ge \|\beta(x^k)\|$. In what follows, we prefer (18) as it simplifies the error estimates.

Now we are ready to describe the basic algorithm in the form that is convenient for the analysis.

Algorithm 1 differs from that proposed by Kučera in three points. First, it implements all the changes of the working set by means of the gradient projection steps, so that the active variables change whenever the active set is updated. Second, it uses the superrelaxation. Finally, it uses a different test to decide the next step.

Mathematical programming. 2012, vol. 135, no. 1-2, p. 195-220. http://dx.doi.org/10.1007/s10107-011-0454-2



**Algorithm 1 Modified proportioning with gradient projections (MPGP schema).**

| | |
|---|---|
| | *Given a symmetric positive definite matrix* $A \in \mathbb{R}^{n\times n}$ *and an* $n$*-vector* $b$*. Choose* $x^0 \in \Omega$ *and* $\overline{\alpha} \in (0, 2\|A\|^{-1})$*. For* $k = 0, 1, \ldots$ *choose* $x^{k+1}$ *by the following rules:* |
| *(i)* | *If* $g^P(x^k) = o$*, set* $x^{k+1} = x^k$*.* |
| *(ii)* | *If* $x^k$ *is proportional and* $g^P(x^k) \neq o$*, try to generate* $x^{k+1}$ *by the conjugate gradient step. If* $x^{k+1} \in \Omega$*, then accept it, else generate* $x^{k+1}$ *by the gradient projection step.* |
| *(iii)* | *If* $x^k$ *is not proportional, define* $x^{k+1}$ *by the gradient projection step.* |

The performance of MPGP can be improved by enhancing the feasible half-step introduced in [20]. This modification of our earlier MPGP algorithm for bound constrained problems [13] is based on a simple observation that the gradient can be updated at any point on the conjugate gradient path without a matrix–vector multiplication, so that the gradient projection can be carried out at nearly the same cost from the nearest point of the boundary of $\Omega$ to the current iterate in the conjugate gradient direction rather than from the current iterate. Since our analysis is based on the worst case analysis, the implementation of the feasible half-step does not result in improving the error bounds, but it improves the performance of MPGP due to the additional decrease of the cost function obtained just for a few scalar products. See also the book [13]. The MPGP algorithm with a feasible half-step reads as follows.

## 5 Error bounds

In this section, we give bounds on the difference between the value of the cost function at the solution and the current iterate. These bounds guarantee an R–linear rate of convergence in the extreme eigenvalues of the Hessian of the cost function that is independent of the constraints. We shall use some well established results.

**Lemma 3** *Let* $\Omega$ *be a closed convex set, let* $\widehat{x}$ *denote the unique solution of* (1)*, let* $\lambda_1$ *denote the smallest eigenvalue of* $A$*,* $x \in \Omega$*, and* $g = Ax - b$*. Then the following statements hold:*
*(i) If* $0 < \alpha \leq \|A\|^{-1}$*, then*

$$f\big(P_\Omega\,(x - \alpha g)\big) - f(\widehat{x}) \leq \nu(\alpha)\big(f(x) - f(\widehat{x})\big), \tag{20}$$

*where*

$$\nu(\alpha) = 1 - \alpha\lambda_1.$$

*(ii) If* $\Omega$ *is subsymmetric and* $\|A\|^{-1} < \alpha \leq 2\|A\|^{-1}$*, then*

$$f\big(P_\Omega\,(x - \alpha g)\big) - f(\widehat{x}) \leq \nu(\alpha)\big(f(x) - f(\widehat{x})\big), \tag{21}$$

*where*

$$\nu(\alpha) = 1 - \widehat{\alpha}\lambda_1, \quad \widehat{\alpha} = 2\|A\|^{-1} - \alpha.$$

*Proof* (i) Replace $f$ by $\alpha f$ in the statement and the proof of Theorem 4.1 of [20]. Though Theorem 4.1 of [20] is formulated for bound constraints, its proof exploits only the convexity of $\Omega$ and is valid also for (1). See also the proof of Lemma 5.9 in [13].
(ii) See Theorem 4.2 of Bouchala, Dostál, and Vodstrčil [5].

**Algorithm 2 MPGP with a feasible half-step.**

*Given a symmetric positive definite matrix* $A \in \mathbb{R}^{n\times n}$, $b \in \mathbb{R}^n$, *and* $\Omega$.
*Step 0.* { *Initialization of parameters.*}
*Choose* $x^0 \in \Omega$, $\overline{\alpha} \in (0, 2\|A\|^{-1})$, $\delta \in (0, 1/2]$, *and the relative stopping tolerance* $\varepsilon > 0$. *Set* $k = 0$, $g = Ax^0 - b$, $p = \varphi(x^0)$.

**if** $2\delta g^T g^P \le \|\varphi(x^k)\|^2$
*Step 1.* {*Proportional* $x^k$. *Trial conjugate gradient step.*}
$\alpha_{cg} = g^T p / p^T A p$
$\alpha_f = \max\{\alpha : x^k - \alpha p \in \Omega\}$
**if** $\alpha_{cg} \le \alpha_f$
*Step 2.* { *Conjugate gradient step.*}
$x^{k+1} = x^k - \alpha_{cg} p, \; g = g - \alpha_{cg} A p$
$\gamma = \varphi\left(x^{k+1}\right)^T Ap / p^T A p, \; p = \varphi\left(x^{k+1}\right) - \gamma p$
**else**
*Step 3.* {*Gradient projection step with halfstep.*}
$x^{k+\frac{1}{2}} = x^k - \alpha_f p, \; g = g - \alpha_f A p$
$x^{k+1} = P_\Omega\left(x^{k+\frac{1}{2}} - \overline{\alpha} g\right)$
$g = Ax^{k+1} - b, \; p = \varphi\left(x^{k+1}\right)$
**end if**
**else**
*Step 4.* {*Gradient projection step.*}
$x^{k+1} = P_\Omega\left(x^k - \overline{\alpha} g\right)$
$g = Ax^{k+1} - b, \; p = \varphi\left(x^{k+1}\right)$
**end if**
$k = k + 1$
**end while**
*Step 5.* {*Return (possibly inexact) solution.*}
$\widetilde{x} = x^k$

We shall need also the inequalities formulated in the following lemma.

**Lemma 4** *Let* $x \in \Omega$ *and* $\alpha > 0$ *and let us denote* $g = g(x) = Ax - b$, $\widetilde{g} = \widetilde{g}_\alpha(x)$, *and* $g^P = g^P(x)$. *Then*

$$\|\widetilde{g}\|^2 \le \widetilde{g}^T g \le \|g\|^2. \tag{22}$$

*and*

$$g^T \widetilde{g} \le g^T g^P = \|g^P\|^2. \tag{23}$$

*Proof* Using $x \in \Omega$, $y \in \mathbb{R}^n$,

$$\left(x - P_\Omega(y)\right)^T \left(y - P_\Omega(y)\right) \le 0,$$

we get for any $\alpha > 0$ and $y = x - \alpha g$

$$\alpha \widetilde{g}^T(-\alpha g + \alpha \widetilde{g}) = \left(x - (x - \alpha \widetilde{g})\right)^T \left(x - \alpha g - (x - \alpha \widetilde{g})\right) \le 0.$$

After simple manipulations, we get (22).

To prove (23), notice that $x - g^P$ is the projection of $x - g$ to the set

$$\hat{\Omega} = \hat{\Omega}_1 \times \cdots \times \hat{\Omega}_s,$$

Mathematical programming. 2012, vol. 135, no. 1-2, p. 195-220. http://dx.doi.org/10.1007/s10107-011-0454-2



where

$$\begin{aligned} &\hat{\Omega}_i = \{\mathbf{y}_i \in \mathbb{R}^{\ell_i} : \hat{h}_i(\mathbf{y}_i) \le 0\}, \\ &\hat{h}_i(\mathbf{y}_i) = (\mathbf{y}_i - \mathbf{x}_i)^T \nabla h_i(\mathbf{x}_i) \qquad \text{for } i \in \mathcal{A}(x), \\ &\hat{h}_i(\mathbf{y}_i) = -1 \qquad\qquad\qquad\qquad\quad \text{for } i \in \mathcal{F}(x). \end{aligned}$$

Since $x - \widetilde{g}$ is the projection of $x - g$ to $\Omega$ and $\Omega \subseteq \hat{\Omega}$, we have $x - \widetilde{g} \in \Omega$ and

$$\|g - g^P\|^2 = \|(x-g) - (x - g^P)\|^2 \le \|(x-g) - (x - \widetilde{g})\|^2 = \|g - \widetilde{g}\|^2.$$

It follows that

$$-2g^T g^P + \|g^P\|^2 \le -2g^T \widetilde{g} + \|\widetilde{g}\|^2.$$

To finish the proof, it is enough to observe that $g^T g^P = \|g^P\|^2$ by (8) and use (22).

Now we are prepared to begin the convergence analysis of our MPGP algorithm.

**Theorem 1** *Let $\Omega$ be a closed convex set, let $\widehat{x}$ denote the unique solution of (1), let $\lambda_1$ denote the smallest eigenvalue of $A$, and let $\{x^i\}$ be generated by Algorithm 1 with $x^0 \in \Omega$, $\alpha \in (0, 2\|A\|^{-1})$, and $\delta \in (0, 1/2]$. Then the following statements hold:*
*(i) If $0 < \alpha \le \|A\|^{-1}$, then for any $k \ge 0$*

$$f\big(x^{k+1}\big) - f(\widehat{x}) \le \eta(\alpha)\big(f(x^k) - f(\widehat{x})\big), \tag{24}$$

*where*

$$\eta(\alpha) = 1 - \delta\alpha\lambda_1.$$

*(ii) If $\Omega$ is subsymmetric and $\|A\|^{-1} \le \alpha \le 2\|A\|^{-1}$, then*

$$f\big(x^{k+1}\big) - f(\widehat{x}) \le \eta(\alpha)\big(f(x^k) - f(\widehat{x})\big), \tag{25}$$

*where*

$$\eta(\alpha) = 1 - \frac{1}{2}\delta\widehat{\alpha}\lambda_1, \quad \widehat{\alpha} = 2\|A\|^{-1} - \alpha. \tag{26}$$

*Proof* First observe that if $x^{k+1}$ is generated by the gradient projection step, then the estimates of Theorem 1 are satisfied by Lemma 3. Thus it is enough to estimate the decrease of the cost function for the conjugate gradient step.
*(i)* Let us assume that $x^{k+1}$ is generated by the conjugate gradient step (13), so that $x^k$ is proportional (18). Using (15), (18), (23), and simple manipulations, we get

$$\begin{aligned} f(x^{k+1}) &\le f\left(x^k - \alpha_{cg}\varphi(x^k)\right) = f(x^k) - \frac{1}{2}\frac{\|\varphi(x^k)\|^4}{\varphi(x^k)^T A \varphi(x^k)} \\ &\le f(x^k) - \frac{1}{2}\alpha\|\varphi(x^k)\|^2 \le f(x^k) - \delta\alpha g^T(x^k) g^P(x^k) \\ &\le f(x^k) - \delta\alpha\widetilde{g}_\alpha^T(x^k) g(x^k) \\ &\le \delta\big(f(x^k) - \alpha\widetilde{g}_\alpha^T(x^k)g(x^k) + \frac{\alpha^2}{2}\widetilde{g}_\alpha^T(x^k)A\widetilde{g}_\alpha(x^k)\big) + (1-\delta)f(x^k) \\ &= \delta f\Big(P_\Omega\big(x^k - \alpha g(x^k)\big)\Big) + (1-\delta)f(x^k). \end{aligned}$$

After subtracting $f(\widehat{x})$ from the first and the last expression and using (20), we get

$$\begin{aligned} f(x^{k+1}) - f(\widehat{x}) &\le \delta\left(f\Big(P_\Omega\big(x^k - \alpha g(x^k)\big)\Big) - f(\widehat{x})\right) + (1-\delta)\big(f(x^k) - f(\widehat{x})\big) \\ &\le \big(\delta\nu(\alpha) + 1 - \delta\big)\Big(f\big(x^k\big) - f(\widehat{x})\Big). \end{aligned}$$

Substituting $\nu(\alpha)$ from (20) we get (24).

Mathematical programming. 2012, vol. 135, no. 1-2, p. 195-220. http://dx.doi.org/10.1007/s10107-011-0454-2



*(ii)* It is enough to modify the above chain of relations by using

$$f(x^k) - \frac{1}{2}\frac{\|\varphi(x^k)\|^4}{\varphi(x^k)^T A\varphi(x^k)} \leq f(x^k) - \frac{1}{4}\alpha\|\varphi(x^k)\|^2. \tag{27}$$

## 6 Bound on the norm of the projected gradient

To use the MPGP algorithm in the inner loops of other algorithms, we must be able *to recognize* when we are near the solution. However, there is a catch – though by Lemma 2 the latter can be tested by a norm of the projected gradient, Theorem 1 does not guarantee that such test is positive near the solution. The projected gradient is not a continuous function of the iterates! Thus if $x^0 \in \Omega$ is an approximation of the solution, it is impossible to give a bound on the norm of $g^P(x^0)$ in terms of the cost function error.

Here we show that the situation is different for the subsequent iterates of MPGP. To see why, let us assume that $\{x^k\}$ is generated by MPGP for the solution of (1) and let $k \geq 1$ be arbitrary but fixed. The main tool in our analysis is the linearized problem associated with $x^k$ that reads

$$\text{minimize } f(x) \quad \text{subject to} \quad x \in \hat{\Omega}_1^k \times \cdots \times \hat{\Omega}_s^k, \tag{28}$$

where

$$\begin{aligned} &\hat{\Omega}_i^k = \{\mathbf{x}_i \in \mathbb{R}^{\ell_i} : \hat{h}_i(\mathbf{x}_i) \leq 0\}, \\ &\hat{h}_i(\mathbf{x}_i) = (\mathbf{x}_i - \mathbf{x}_i^k)^T \nabla h_i(\mathbf{x}_i^k) \qquad \text{for } i \in \mathcal{A}(x^k), \\ &\hat{h}_i(\mathbf{x}_i) = -1 \qquad\qquad\qquad\qquad\quad\; \text{for } i \in \mathcal{F}(x^k). \end{aligned}$$

Comparing problem (28) with our original problem (1), we can see that the original constraints on $\mathbf{x}_i$ are omitted in (28) for $i \in \mathcal{F}(x^k)$ and replaced by their linearized versions for $i \in \mathcal{A}(x^k)$. Since $h_i$ are convex by assumptions, we get easily

$$\Omega \subseteq \hat{\Omega} \text{ and } \mathbf{n}_i = \hat{\mathbf{n}}_i \ \forall i \in \mathcal{A}(x^k). \tag{29}$$

Problem (28) is defined so that the iterate $x^k$, which was by the assumption obtained from $x^{k-1}$ by the MPGP algorithm for the solution of problem (1), can also be considered as an iterate for the solution of problem (28). Let us mention that for the bound constrained problems, this observation was used first in [20]. Kučera adapted this observation for the proof of convergence of his K-gradient [19].

We use the hat to distinguish the concepts related to problem (28) from those related to our original problem (1) where necessary. For example, $\hat{\mathcal{A}}(x)$ denotes the active set of $x \in \mathbb{R}^n$. For typographical reasons, we denote the reduced gradient for (28) by $\hat{g}_\alpha$. The following relations are important in what follows.

**Lemma 5** *Let $x^k$ denote an iterate generated by the MPGP algorithm under the assumptions of Theorem 1, let problem* (28) *be associated with $x^k$, and let $\hat{g}^P(x^k)$ and $\hat{g}_\alpha(x^k)$ denote the projected gradient and the reduced gradient associated with problem* (28)*, respectively. Then*

$$g^P(x^k) = \hat{g}^P(x^k) = \hat{g}_\alpha(x^k). \tag{30}$$

Mathematical programming. 2012, vol. 135, no. 1-2, p. 195-220. http://dx.doi.org/10.1007/s10107-011-0454-2



*Proof* Let $i \in \mathcal{A}(x^k)$, $n = n(x^k)$, $g = g(x^k)$, $\alpha > 0$, $\hat{g} = \hat{g}_\alpha(x^k)$, and $\mathbf{n}_i^T \mathbf{g}_i < 0$. Using the standard linear algebra, we get

$$\mathbf{x}_i^k - P_{\hat{\Omega}_i}(\mathbf{x}_i^k - \alpha \mathbf{g}_i) = \alpha \hat{\mathbf{g}}_i = \alpha \mathbf{g}_i - \alpha\{\mathbf{n}_i^T \mathbf{g}_i\}^- \mathbf{n}_i = \alpha \mathbf{g}_i - \alpha\{\hat{\mathbf{n}}_i^T \mathbf{g}_i\}^- \hat{\mathbf{n}}_i.$$

Thus $\alpha \hat{\mathbf{g}}_i = \alpha \mathbf{g}_i^P = \alpha \hat{\mathbf{g}}_i^P$. If $i \in \mathcal{F}(x^k)$ or $\mathbf{n}_i^T \mathbf{g}_i \geq 0$, then obviously $\mathbf{g}_i^P = \hat{\mathbf{g}}_i^P = \hat{\mathbf{g}}_i = \mathbf{g}_i$.

We shall use also the following lemma which is due to Kučera [19].

**Lemma 6** *Let $\xi^0$, $\xi^1$, and $\xi^2$ belong to $\hat{\Omega}$ and satisfy*

$$f(\xi^2) - f(\widehat{\xi}) \leq \eta\big(f(\xi^1) - f(\widehat{\xi})\big) \leq \eta^2\big(f(\xi^0) - f(\widehat{\xi})\big), \tag{31}$$

*where $\widehat{\xi}$ denote the solution of* (28) *and*

$$\eta \in (0, 1).$$

*Then*

$$f(\xi^1) - f(\xi^2) \leq \frac{1+\eta}{1-\eta}\eta\left(f(\xi^0) - f(\xi^1)\right).$$

*Proof* See [19].

Now we are ready to prove the main result of this section.

**Theorem 2** *Let $\{x^k\}$ denote the iterates generated by the MPGP algorithm under the assumptions of Theorem 1. Then for any $k \geq 1$*

$$\|g^P(x^k)\|^2 \leq \frac{2\big(1+\eta\big)}{\widehat{\alpha}\big(1-\eta\big)}\eta^k\big(f(x^0) - f(\widehat{x})\big), \tag{32}$$

*where $\eta = \eta(\alpha)$ is defined in Theorem 1 and $\widehat{\alpha} = \min\big\{\alpha, 2\|A\|^{-1} - \alpha\big\}$.*

*Proof* As we have mentioned above, our main tool is the observation that given a $k \geq 1$, we can consider iterates $x^{k-1}$ and $x^k$ as initial iterates for our auxiliary problem (28). Let us show that

$$f(x^k) - f(\widehat{\xi}) \leq \eta(\alpha)\big(f(x^{k-1}) - f(\widehat{\xi})\big), \tag{33}$$

where $\widehat{\xi}$ denotes a unique solution of (28).

Let us first assume that $x^k$ is generated by the conjugate gradient step for problem (1), so that $\mathbf{x}_i^k = \mathbf{x}_i^{k-1}$ for $i \in \mathcal{A}(x^{k-1})$. Since problem (28) is defined so that $\mathcal{A}(x^k) = \hat{\mathcal{A}}(x^k)$, it follows that $\hat{\mathcal{A}}(x^{k-1}) \supseteq \mathcal{A}(x^{k-1})$. Noticing that $\hat{\mathcal{A}}(x) \subseteq \mathcal{A}(x)$ for any $x \in \Omega$, we get

$$\hat{\mathcal{A}}(x^{k-1}) = \mathcal{A}(x^{k-1}).$$

Thus $\hat{\varphi}(x^{k-1}) = \varphi(x^{k-1})$. Since $g^P(x^{k-1}) = \hat{g}^P(x^{k-1})$ by Lemma 5, it follows that $x^{k-1}$ is proportional also as an iterate for the solution of problem (28) and (33) holds true by Theorem 1.

To prove (33) for $x^k$ generated by the gradient projection step, notice that $\hat{\Omega}$ is defined in such a way that

$$x^k = P_\Omega\big(x^{k-1} - \alpha g(x^{k-1})\big) = P_{\hat{\Omega}}\big(x^{k-1} - \alpha g(x^{k-1})\big).$$

Thus (33) holds true by Theorem 1. We conclude that (33) holds true.

Let us define

$$\xi^0 = x^{k-1},\ \xi^1 = x^k, \quad \text{and} \quad \xi^2 = P_{\hat{\Omega}}\big(\xi^1 - \alpha g(\xi^1)\big).$$

Using Theorem 1 and (33), we get

$$\big(f(\xi^2) - f(\widehat{\xi})\big) \le \eta(\alpha)\big(f(\xi^1) - f(\widehat{\xi})\big) \le \eta(\alpha)^2\big(f(\xi^0) - f(\widehat{\xi})\big). \tag{34}$$

Thus the assumptions of Lemma 6 are satisfied with $\eta = \eta(\alpha)$ and

$$\begin{aligned} f(\xi^1) - f(\xi^2) &\le \frac{1+\eta}{1-\eta}\eta\left(f(\xi^0) - f(\xi^1)\right) \\ &= \frac{1+\eta}{1-\eta}\eta\left(f(x^{k-1}) - f(x^k)\right) \\ &\le \frac{1+\eta}{1-\eta}\eta\left(f(x^{k-1}) - f(\widehat{x})\right) \\ &\le \frac{1+\eta}{1-\eta}\eta^k\left(f(x^0) - f(\widehat{x})\right). \end{aligned}$$

Finally, using Lemma 5, relations (8), and simple manipulations, we get

$$\begin{aligned} f\left(\xi^1\right) - f\left(\xi^2\right) &= f\left(\xi^1\right) - f\big(P_{\hat{\Omega}}(\xi^1 - \alpha g(\xi^1))\big) \\ &= \alpha\hat{g}_\alpha^T(\xi^1)g(\xi^1) - \frac{\alpha^2}{2}\hat{g}_\alpha^T(\xi^1)A\hat{g}_\alpha(\xi^1) \\ &\ge \alpha\hat{g}_\alpha^T(\xi^1)g(\xi^1) - \frac{\alpha^2}{2}\|\hat{g}_\alpha(\xi^1)\|^2\|A\| \\ &= (\alpha - \frac{\alpha^2}{2}\|A\|)\,\hat{g}_\alpha^T(\xi^1)g(\xi^1) \\ &= \frac{1}{2}\|A\|\alpha(2\|A\|^{-1} - \alpha)\,\hat{g}_\alpha^T(\xi^1)g(\xi^1) \\ &\ge \frac{\widehat{\alpha}}{2}\hat{g}_\alpha^T(\xi^1)g(\xi^1) = \frac{\widehat{\alpha}}{2}\left(\hat{g}^P(\xi^1)\right)^T g(\xi^1) \\ &= \frac{\widehat{\alpha}}{2}\|\hat{g}^P(\xi^1)\|^2 = \frac{\widehat{\alpha}}{2}\|g^P(\xi^1)\|^2 = \frac{\widehat{\alpha}}{2}\|g^P(x^k)\|^2. \end{aligned}$$

To check directly the last inequality, consider separately $\alpha \in (0, \|A\|^{-1}]$ and $\alpha \in (\|A\|^{-1}, 2\|A\|^{-1}]$. Putting the last terms of above chains of relations together, we get (32).

## 7 Separable and equality constraints

The bound on the projected gradient given in Section 6 enables us to plug the MPGP algorithm into our SMALSE-M (semimonotonic augmented Lagrangian for separable and equality constrained QP problems) algorithm for the solution of the problem to find the minimizer of a strictly convex quadratic function subject to separable convex inequality and linear equality constraints, that is,

$$\text{minimize } f(x) \quad \text{subject to} \quad x \in \Omega_{SE} \tag{35}$$

with

$$\Omega_{SE} = \{x \in \Omega :\ Cx = o\}, \tag{36}$$

Mathematical programming. 2012, vol. 135, no. 1-2, p. 195-220. http://dx.doi.org/10.1007/s10107-011-0454-2



where $C \in \mathbb{R}^{m \times n}$ and $\Omega$ is the feasible set of problem (1). We suppose that $\Omega_{SE}$ is non-empty and admit dependent rows of $C$.

The SMALSE-M is a Uzawa-type algorithm which generates approximations for the Lagrange multipliers $\lambda \in \mathbb{R}^m$ in the outer loop and solves auxiliary problems with separable constraints in the inner loop.

To describe SMALSE-M, let us introduce the augmented Lagrangian $L(x, \lambda, \varrho)$ for problem (35) by

$$L(x, \lambda, \varrho) \;=\; \frac{1}{2} x^T (A + \varrho C^T C) x \;-\; x^T b \;+\; \lambda^T C x,$$

so that its gradient is given by

$$g(x, \lambda, \varrho) \;=\; \nabla_x L(x, \lambda, \varrho) \;=\; (A + \varrho C^T C) x \;-\; b \;+\; C^T \lambda.$$

Our algorithm reads as follows.

**Algorithm 3 Semimonotonic augmented Lagrangians (SMALSE-M).**

*Given a symmetric positive definite matrix* $A \in \mathbb{R}^{n \times n}$, $C \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^n$, $\Omega$.
*Step 0.* {*Initialization.*}
  *Choose* $\eta > 0,\; \beta > 1,\; M_0 > 0,\; \varrho > 0,\; \lambda^0 \in \mathbb{R}^m$
  **for** $k = 0, 1, 2, \ldots$
*Step 1.* {*Inner iteration with adaptive precision control.*}
  *Find* $x^k \in \Omega$ *such that*

$$\|g^P(x^k, \lambda^k, \varrho)\| \le \min\{M_k \|Cx^k\|, \eta\} \tag{37}$$

*Step 3.* {*Updating the Lagrange multipliers.*}

$$\lambda^{k+1} = \lambda^k + \varrho C x^k \tag{38}$$

*Step 4.* {*Update* $M$ *provided the increase of the Lagrangian is not sufficient.*}
  **if** $k > 0$ **and** $L(x^k, \lambda^k, \varrho) < L(x^{k-1}, \lambda^{k-1}, \varrho) + \frac{\varrho}{2}\|Cx^k\|^2$
    $M_{k+1} = M_k / \beta$
  **else**
    $M_{k+1} = M_k$
  **end** if
  **end** for

*Step 1* may be implemented by any algorithm for minimization of the augmented Lagrangian $L$ with respect to $x$ subject to the separable constraints that guarantees convergence of the projected gradient to zero. It follows by Theorem 2 that we can use our MPGP algorithm.

The SMALSE-M algorithm is formally identical with its predecessor SMALBE-M (semimonotonic augmented Lagrangians for bound and equality constraints) introduced in [13]; the theory is the same due to Lemma 1 and some other relations proved

Mathematical programming. 2012, vol. 135, no. 1-2, p. 195-220. http://dx.doi.org/10.1007/s10107-011-0454-2



above. Let us recall that SMALBE-M is a modification of the SMALBE algorithm introduced in [10] and [11] which keeps the balancing parameter $M$ constant and controls the regularization parameter $\varrho$. The algorithm SMALBE-M has been used successfully in the development of a scalable algorithm for the solution of frictionless problems [18]. Its development originates from the algorithm proposed by Conn, Gould, and Toint [7] for identifying stationary points of more general problems. Its early modification by Dostál, Friedlander, and Santos [15] was used by Dostál and Horák to develop a FETI based algorithm with experimental evidence of its scalability [16].

A unique feature of SMALSE-M, inherited from SMALBE-M, is its optimality, i.e., its capability to find an approximate solution of problem (35) in a number of steps which is uniformly bounded in terms of the bounds on the spectrum of $A + \varrho C^T C$. It has been also proved that if

$$\varrho \lambda_{\min}(A) \geq M_k^2,$$

then there is no update of the balancing parameter $M_k$. It simply follows that

$$M_k^2 \geq \min\{M_0^2, \varrho\lambda_{\min}(A)/\beta^2\}.$$

To present explicitly the optimality result, let $\mathcal{T}$ denote any set of indices and let for any $t \in \mathcal{T}$ be defined a problem

$$\text{minimize} \quad f_t(x) \quad \text{subject to} \quad x \in \Omega^t \tag{39}$$

with $f_t(x) = \frac{1}{2}x^T A_t x - b_t^T x$, $A_t \in \mathbb{R}^{n_t \times n_t}$ symmetric positive definite, $b_t \in \mathbb{R}^{n_t}$, and

$$\Omega^t = \{x \in \mathbb{R}^{n_t} : C_t x = 0,\ h_1^t(\mathbf{x}_1) \leq 0, \ldots,\ h_{s^t}^t(\mathbf{x}_{s^t}) \leq 0\},$$

where $C_t \in \mathbb{R}^{m_t \times n_t}$, $h_i^t : \mathbb{R}^{n_i^t} \mapsto \mathbb{R}$ are continuously differentiable convex functions and $\mathbf{x}_i \in \mathbb{R}^{\ell_i^t}$ denotes the $i$-th segment of $x_t \in \mathbb{R}^{n_t}$ so that $x_t = x = (\mathbf{x}_1^T, \ldots, \mathbf{x}_{s^t}^T)^T$, $\sum_{i=1}^{s^t} \ell_i^t = n_t$. Finally, we assume that $o \in \Omega^t$. The optimality result reads as follows.

**Theorem 3** *Let*

$$0 < \varepsilon < 1, \quad 0 < a_{\min} < a_{\max}, \quad \textit{and} \quad 0 < c_{\max}$$

*be given constants and let the class of problems (39) satisfy*

$$a_{\min} \leq \lambda_{\min}(A_t) \leq \lambda_{\max}(A_t) \leq a_{\max} \quad \textit{and} \quad \|C_t\| \leq c_{\max}. \tag{40}$$

*Let $\{x_t^k\}, \{\lambda_t^k\}$, and $\{M_{t,k}\}$ be generated by Algorithm 3 (SMALSE-M) for (39) with*

$$\|b_t\| \geq \eta_t \geq \varepsilon\|b_t\|,\ \beta > 1,\ \varrho > 0,\ M_{t,0} = M_0 > 0, \quad \textit{and} \quad \lambda_t^0 = o.$$

*Let Step 1 of Algorithm 3 be implemented by Algorithm 1 (MPGP) in order to generate the iterates $x_t^{k,0}, x_t^{k,1}, \ldots, x_t^{k,l} = x_t^k$ for the solution of (39) starting from $x_t^{k,0} = x_t^{k-1}$ with $x_t^{-1} = o$, where $l = l_{t,k}$ is the first index satisfying*

$$\|g_t^P(x_t^{k,l}, \lambda_t^k, \varrho)\| \leq \min\{M_{t,k}\|C_t x_t^{k,l}\|, \eta_t\}. \tag{41}$$

*Then Algorithm 3 generates an approximate solution $x_t^{k_t}$ of any problem (39) which satisfies*

$$\|g_t^P(x_t^{k_t}, \lambda_t^{k_t}, \varrho)\| \leq M_0\varepsilon\|b_t\| \quad \textit{and} \quad \|C_t x_t^{k_t}\| \leq \varepsilon\|b_t\| \tag{42}$$

*at $O(1)$ inner iterations.*

*Proof* Since our generalization of the projected gradient satisfies all the essential inequalities used in the proof of optimality of SMALBE-M with the inner loop implemented by the MPRGP algorithm, it follows that the proof of Theorem 3 is formally identical to the proof of optimality of SMALBE-M with the inner loop implemented by the MPRGP (see Chapter 5 of the book [13]). Alternatively, it is possible to observe that the K-gradient $g^K$ of Kučera satisfies

$$\|g^P(x)\| \leq \|g^K(x)\| \leq 2\|g^P(x)\|$$

and use Theorem 9.2 of Dostál and Kučera [19].

## 8 Numerical experiments

The algorithms described above were implemented in `MatSol` library [33] developed in Matlab environment and parallelized using Matlab Distributed Computing Engine produced by MathWorks company. For the computations we used the HP Blade system, model BLc7000 with one master node and eight computational nodes, each with two dual core CPUs AMD Opteron 2210 HE. All the computations were carried out with the parameters: $M_0 = 1$, $\eta = \|b\|$, $\varrho \approx \|A\|$, $\delta = 0.25$, $\overline{\alpha} \approx 2\|A\|^{-1}$, $\beta = 10$, $x^0 = o$, $\lambda^0 = o$,

We tested the performance of our algorithms on the solution of a 3D contact problem of two cantilever beams in mutual contact with the Tresca friction. Each beam is represented by a steel box $2000 \times 1000 \times 1000$ [mm]. The geometry with the imposed boundary conditions and material properties are specified in Fig. 2 and the slip bound $\Psi = 10$ [MPa].

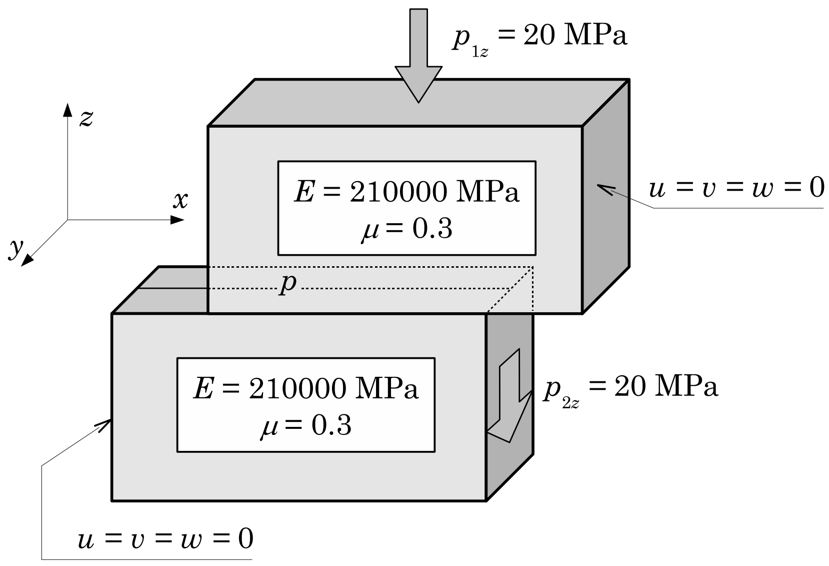


**Fig. 2** Model specification

In Table 1, we see the dependence of the number of Hessian multiplications on the parameters $\overline{\alpha}$ and $\delta$. The results show that the superrelaxation improves the performance of the algorithm in agreement with the theory (see, e.g., Bertsekas [3] or Dostál [13]) and that the performance of MPGP is not sensitive to the choice of $\delta$, at least sufficiently far from extreme values.

**Table 1** Hessian multiplications (full cg steps/halfsteps) for varying $\overline{\alpha}$ and $\delta$ – no decomposition.

| $\delta$ | $\overline{\alpha} = 0.5\|A\|^{-1}$ | $1.0\|A\|^{-1}$ | $1.5\|A\|^{-1}$ | $1.7\|A\|^{-1}$ | $1.9\|A\|^{-1}$ | $1.99\|A\|^{-1}$ |
|---|---|---|---|---|---|---|
| 0.01 | 269(16/63) | 183(17/49) | 137(16/36) | 123(15/32) | 127(16/37) | 120(16/33) |
| 0.10 | 261(9/62) | 177(7/50) | 125(8/33) | 119(8/33) | 118(8/34) | 108(8/30) |
| 0.25 | 268(5/55) | 181(5/50) | 127(5/33) | 118(4/32) | 117(5/34) | 106(6/28) |
| 0.40 | 273(2/55) | 189(0/49) | 133(0/34) | 122(0/32) | 122(0/35) | 109(0/29) |
| 0.50 | 1,016(0/3) | 517(0/1) | 350(0/1) | 310(0/0) | 280(0/1) | 268(0/1) |

To demonstrate the power of our algorithms, we give also the results of the above problem solved by the TFETI (total finite element tearing and interconnecting) based domain decomposition method. The method uses a decomposition of the physical domain into subdomains and the finite element discretization characterized by the decomposition and discretization parameters $H$ and $h$, respectively. See Fig. 3.

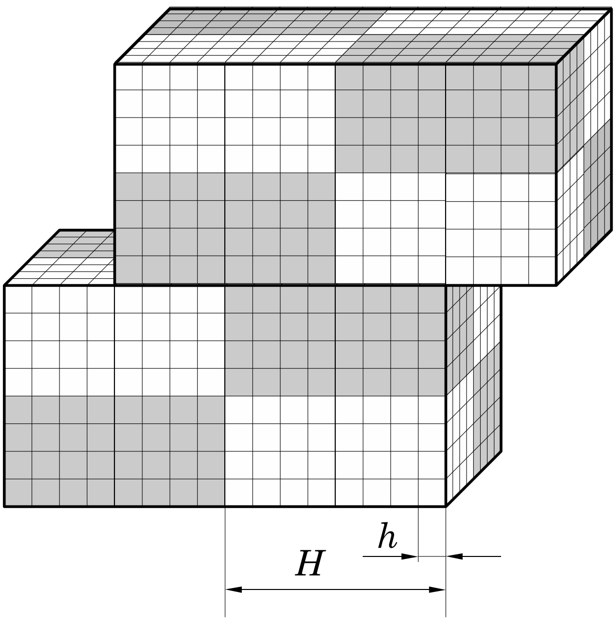


**Fig. 3** Uniform domain decomposition and finite element discretization

Here MPGP is used in the inner loop of the SMALSE-M algorithm. For each $h$ and $H$, the bodies were discretized by structured grids decomposed into the subdomains (see Fig. 3). We kept $H/h = 16$, so that the spectrum of the Hessian matrix is uniformly bounded by the theory of the domain decomposition methods (see [17]). The results for the Tresca friction with the slip bound $\Psi = 10$ [MPa] are reported in Table 2. We can observe that the number of matrix–vector multiplications increases only mildly in agreement with the theory. Industrial application can be found in [17].

**Table 2** Numerical scalability: Tresca friction with TFETI domain decomposition

| Number of subdomains<br>Number of CPUs | $(2 \cdot 2^3)$ 16<br>16 | $(2 \cdot 4^3)$ 128<br>24 | $(2 \cdot 6^3)$ 432<br>24 | $(2 \cdot 8^3)$ 1,024<br>24 |
|---|---|---|---|---|
| Primal variables | 66,096 | 528,768 | 1,784,592 | 4,230,144 |
| Dual variables | 11,883 | 115,443 | 412,347 | 1,004,259 |
| Number of bound constraints | 425 | 1,617 | 3,577 | 6,305 |
| Number of spherical constraints | 425 | 1,617 | 3,577 | 6,305 |
| Number of equality constraints | 96 | 768 | 2,592 | 6,144 |
| SMALSE-M iterations | 11 | 10 | 8 | 11 |
| Hessian multiplications | 135 | 254 | 339 | 371 |
| Solution time [sec] | 28 | 289 | 1,245 | 3,854 |
| Total time [sec] | 33 | 330 | 1,500 | 6,100 |

## 9 Comments and conclusions

We have presented a new algorithm for minimization of a strictly convex quadratic function subject to convex separable inequality constraints. The algorithm is a modification of our earlier algorithms for the solution of bound constrained problem, but it takes into accounts that even a correctly defined active set of the solution does not reduce the problem to the linear one. The estimates presented here are even better than earlier estimates for the bound constraints. However, the estimates are still based on the worst case analysis and do not take into account a possible speedup due to the self-preconditioning property of the conjugate gradient method and some other improvements.

An important feature of this algorithm, which is shared with its predecessors, is an error estimate in terms of bounds on the spectrum of the Hessian matrix of the cost function that is independent of the conditioning of the constraints. If it is applied to a class of problems with the cost functions whose Hessian matrices have the spectrum confined to a given positive interval, the algorithm can find an approximate solution in a uniformly bounded number of basic operations, such as the matrix–vector multiplications. Moreover, if the class of problems admits a sparse representation of the Hessian, it simply follows that the cost of the solution is proportional to the number of unknowns.

Another new feature of our algorithm is using the fixed step gradient projection with superrelaxation. The performance of our algorithm and the effect of superrelaxation is demonstrated on the solution of the contact problem of elasticity with Tresca friction.

Due to the bounds on the projected gradient, the algorithm can be used in the inner loop of the SMALSE-M algorithm for the solution of problems with separable convex constraints and linear equality constraints. The power of MPGP in this context was demonstrated on the solution of a nonlinear problem of mechanics discretized by more than four millions of variables.

Even though it seems that the most important applications are related to the spherical constraints, the whole theory is valid for more general separable convex sub-symmetric constraints. The results that do not consider superrelaxation are valid for any convex separable sets.

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